

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.71

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 5.03e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Disulfoton</div> <div>Measured: 4.02</div> <div>Predicted: 3.71</div>	<div>Image not found</div> <div>Phorate</div> <div>Measured: 3.56</div> <div>Predicted: 3.36</div>	<div>Image not found</div> <div>Terbufos</div> <div>Measured: 4.48</div> <div>Predicted: 4.21</div>
<div>Image not found</div> <div>O-Ethyl S-[2-(ethylsulfanyl)ethyl] ethylphosphonothioate</div> <div>Measured: 2.03</div> <div>Predicted: 2.30</div>		